Genentech
A Member of the Roche Group

September 7, 2016

Dear Dr. Mobley and Dr. Chodera,

Genentech is, a large pharmaceutical company with interests in a wide range of disease areas. Daniel Ortwine is an experienced computational chemist in the Computational Drug Discovery Group within the Chemistry Department at Genentech, and Baiwei Lin works in our Analytical Chemistry group, specializing in measuring physiochemical properties such as aqueous solubility, pKa, and LogD .

We are very excited to be involved in your proposal, "Advancing predictive physical modeling through focused development of model systems to drive new modeling innovations." As you may be aware, we believe physical modeling is poised to have a real impact on the pharmaceutical drug discovery process, but we also believe there are key challenges the field still needs to resolve to achieve this. The work you propose is absolutely vital to facilitate the necessary advancements.

This letter is to confirm that we are willing to host a student who will help collect experimental data to enable new SAMPL physical property prediction challenges to drive the improvement of these methods. We can provide access to equipment necessary for measuring physical properties that are not typically available to academic laboratories, such as the Sirius T3 (for measurement of pKa, logD, and logS), high-throughput automated shake-flask measurements of logD and logP, and automated membrane permeability assays for compounds available from commercial vendors. We have multiple mechanisms available through which these measurements can be performed. Possibilities include sending a student from your laboratories to perform measurements at Genentech as a visiting scientist, and/or sending a student to us as part of our summer internship program. The latter possibility includes a stipend for focused measurement projects like these.

As you are of course aware, we were already able to do something very similar to this for the SAMPL5 challenge, where – via a summer internship program – we hosted Bas Rustenberg, a student from John Chodera's lab, who measured water-cyclohexane log D values which formed half of the SAMPL5 challenge. We believe we will be able to similarly host academic researchers to help generate data for future SAMPL challenges.

Sincerely,

Daniel Ortwine
Principal Scientist
Computational Chemistry

Baiwei Lin
Scientist
Analytical Chemistry